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A Screening Procedure for Assessing the Transport and Degradation of Solid Waste Constituents in Subsurface and Surface Waters

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16. ABSTRACT

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After high and low estimates are established, qualitative descriptors are assigned to describe the transport and persistence of the compound in subsurface and surface waters.

This procedure has been used to evaluate 193 compounds that were projected to be constituents of solid wastes from 75 manufacturing operations. The results of a sensitivity analysis indicate that where individual environmental process descriptions are defined, changes in rates of degradation of an order of magnitude are required to cause a significant number of changes in qualitative descriptors that define the transport and persistence of the compounds assessed.

The results of this application indicate that the procedure provides a means of qualitatively screening organic chemicals when specified process rate data are available. The evaluation of the small number of metals included in this assessment are speculative. Further research is required to adequately screen metals.

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JOURNAL ARTICLE

A SCREENING PROCEDURE FOR ASSESSING THE TRANSPORT AND DEGRADATION OF SOLID WASTE CONSTITUENTS IN SUBSURFACE AND SURFACE WATERS

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Abstract — An evaluation procedure was developed to rapidly screen chemicals for their potential to contaminate both subsurface and surface waters after disposal and subsequent release from landfills and lagoons. The procedure estimates movement and degradation of chemicals based on the physical and chemical properties of the compound and a defined range of environmental conditions that the compound potentially experiences in groundwater and in rivers, ponds, and reservoirs.

After high and low estimates are established, qualitative descriptors are assigned to describe the transport and persistence of the compound in subsurface and surface waters.

This procedure has been used to evaluate 193 compounds that were projected to be constituents of solid wastes from 75 manufacturing operations. The results of a sensitivity analysis indicate that where individual environmental process descriptions are defined, changes in rates of degradation of an order of magnitude are required to cause a significant number of changes in qualitative descriptors that define the transport and persistence of the compounds assessed.

The results of this application indicate that the procedure provides a means of qualitatively screening organic chemicals when specified process rate data are available. The evaluation of the small number of metals included in this assessment are speculative. Further research is required to adequately screen metals.

Keywords — Hazardous waste Transport Degradation Toxic chemicals

Implementation of the National Resource Conservation and Recovery Act (RCRA), the Toxic Substances Control Act (TSCA) and other federal and state regulations has necessitated the development of environmental exposure assessment methods. In many cases, the first task performed in an exposure assessment is a gross screening that defines the scope of the problem and clearly identifies areas that require additional study. This screening analysis is one of the most difficult aspects of performing assessments.

Different screening approaches are required depending upon the purpose of the assessment. When a single toxic substance such as a pesticide or an industrial compound is studied, for example, screening may involve a review of exposure opportunities in terms of a geographical context or in terms of definition of different exposure pathways. In other cases, screening may involve reviews of large numbers of compounds to determine which compounds pose the greatest potential for exposure based upon their transport and degradation properties.

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This paper describes an evaluation procedure that screens large numbers of compounds for their potential to contaminate subsurface and surface waters based upon their physical and chemical properties and a defined range of environmental conditions that the compounds potentially experience. The procedure is qualitative. A range of estimates of the movement and persistence of a particular compound is predicted based upon the variety of environmental conditions at the disposal site. Qualitative descriptors that reflect movement and persistance estimates are then assigned to each compound. These descriptors are subsequently used to evaluate relative exposure potential.

DESCRIPTION OF SCREENING PROCEDURE

The procedure involves two steps: the use of a mathematical model that generates quantitative estimates of exposure and the use of a logic sequence that assigns qualitative descriptors of behavior based on quantitative estimates of exposure. The mathematical model is a simple mass balance technique which routes a pollutant from the point of entry into the environment through a series of typical environments that the pollutant is likely to encounter. All degradation processes considered are assumed to be adequately approximated by a first order rate equation:

$$R_i = k_i * C \tag{1}$$

where

k_i = rate constant for process i
C = concentration of dissolved pollutant
R_i = rate of change in concentration of pollutant due to reaction i

Release rate estimation procedure

In developing the assessment procedure, landfills and lagoons were modeled as sources of contaminants to subsurface and surface waters. These two sources were selected because they are representative of potentially uncontrollable sources. It was assumed that an uncontrolled release from landfills and lagoons will occur, but no detailed description of the nature of the release is included. Rather, the procedure assumes a constant release rate as would be expected from leakage from numerous small or a few large cracks in walls and bottom of the containment facility. Obviously, catastrophic failures are outside the scope of this procedure.

A second major assumption made in estimating the release rate is that transport of a pollutant through soil is not limited by the rate of transport through walls or bottoms of containment facilities. In addition, we assume that the mass of solid waste at the disposal site is sufficiently large to be represented as an infinite source and that the temporal variations in water percolation through the containment walls and bottom do not alter significantly the results of analysis. The assumption that temporal variations are not important is based on the extremely slow subsurface movement of pollutants (on the order of 1 m/yr). Consequently, fluctuations caused by alternating wet and dry weather periods are averaged out over the time frame of interest, which is on the order of 10 to 100 years.

To estimate release rates, solid waste constituents are divided into two categories. The component present in highest concentration is designated as the major constituent. Other components are designated as minor constituents. For the major constituent, the concentration in water leaching out of a disposal site is assumed to be the solubility of the constituent. Thus, assuming no solids movement, the amount emitted per unit surface area of containment is

$$J = \bar{V} * C_s \tag{2}$$

where

C_s = solubility of the major constituent
$\bar{V}$ = volume flowrate of water percolating through the containment site per unit surface area of the containment site.

For minor constituents, the concentration in water leaching out of a containment site is assumed to be the equilibrium concentration obtained by partitioning between solid phase material and dissolved material. Thus, the amount emitted per unit surface area of containment is

$$J = \frac{V \bullet F}{K} \tag{3}$$

where

K = partition coefficient for a pollutant between organic matter and solution
F = fraction of solid waste that is the contaminant of interest

Once the pollutants are released to groundwater, they are transported with groundwater movement and eventually released into surface waters. To estimate this movement, the screening procedure assumes that pollutants move in plug flow from the point of release to the point of entry into surface waters. Since long-term impacts were the primary basis for screening, the procedure also assumes that the soil sorptive capacity has been reached in both unsaturated and saturated soil zones and that steady-state concentration profiles have been achieved. Given these assumptions, a mass balance can be derived that defines the transport and degradation of a pollutant in groundwater as follows:

$$v \frac{\partial C}{\partial x} = - \sum_i k_i \bullet C \tag{4}$$

where

C = concentration of the contaminant in groundwater
x = distance from containment site
v = velocity of groundwater movement

The solution to equation 4 is

$$C/C_o = \exp\left\{ - \sum_i k_i \bullet \frac{x}{v} \right\} \tag{5}$$

where

C/C_o = fraction of mass released from a containment site that reaches a distance x from the site
v = velocity of groundwater movement

In the evaluation of the 193 compounds, hydrolysis was the only degradation process considered in groundwater. This decision was based on the fact that photolysis and light-initiated oxidation reactions do not occur in soils and that bacterial concentrations are usually very low in groundwater. Other reactions can be considered if evidence of occurrence so warrants. Typical concentration profiles predicted by equation 5 are shown in Figure 1. For lagoons, Chow [1] has proposed the following equation for estimation of seepage to adjacent surface water:

$$\hat{V} = \frac{k_h}{2L}(H_1^2 - H_2^2) \tag{6}$$

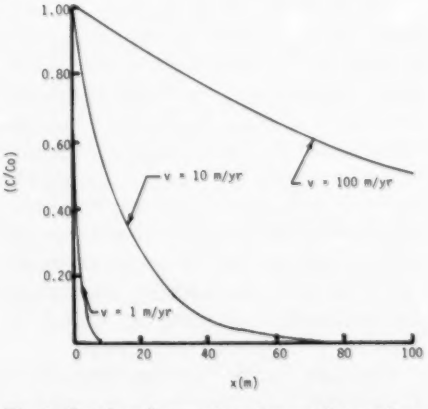

Fig. 1. Fraction of mass released versus distance from point of release $k_{Hyd} = 0.0019$ Day^{-1}

where

$\hat{V}$ = volumetric flow rate of seepage water to surface water per unit length of lagoon adjacent to surface water
k_h = saturated hydraulic conductivity
H_1 = difference in elevation between the lagoon surface and the bottom of the receiving water body
H_2 = depth of the receiving water body
L = distance from containment site to the receiving water body

Water velocity is estimated from the gradient, i.e.,

$$v = \frac{k_h (H_1 - H_2)}{p L}$$

where p is the soil porosity.

Surface water evaluation procedure

Estimating potential contamination of surface waters involves the evaluation of pollutant persistance over a range of environmental conditions. Three types of water bodies — rivers, ponds and reservoirs — are considered. A range of environmental conditions and parameters that potentially affect the fate of pollutants are established for each water body.

For each set of environmental conditions, estimates of the fraction of material emitted that is volatilized to the atmosphere, degraded in the receiving water body, convected out of the water body, bioaccumulated in fish, and sorbed to suspended sediments are made. Finally, for ponds and reservoirs, estimates of the fraction of material emitted that settled with sediment are made. Major degradation processes considered include volatilization, adsorption, bioaccumulation, hydrolysis, photolysis, oxidation and bacterial degradation.

Pollutant sorption to suspended matter in the water body is assumed to obtain an equilibrium partition instantly and to be totally reversible. Furthermore, sorption is assumed to occur only on the organic fraction of the suspended sediment. A linear relationship between the dissolved pollutant concentration and sorbed pollutant concentration is used to describe the partitioning between water and sorbed phases.

$$C' = K * C \tag{7}$$

where

C' = amount of sorbed pollutant per unit mass of sediment
K = sediment / water partition coefficient

Bioaccumulation of the pollutant in fish is assumed to obtain equilibrium partition such that the rate of removal from water can be expressed as

$$R_f = B_f * K^f * C \tag{8}$$

where

K^f = fish tissue / water partition coefficient
B_f = biomass turnover rate

In rivers and water, suspended sediment and pollutant are assumed to move in plug flow. The appropriate partial differential equation that describes pollutant transport and degradation is

$$(1 + K * S) \frac{\partial C}{\partial t} = (1 + K * S) v \frac{\partial C}{\partial x} - \sum_i k_i C \tag{9}$$

For an initial condition $C = C_o$ at $t = o$, equation 4 can be solved to yield:

$$\frac{C}{C_o} = \exp \left\{ - \frac{\sum_i k_i * t}{1 + K * S} \right\} \tag{10}$$

where

v = average velocity of the water
x = distance
S = suspended sediment concentration
t = time of travel

Equation 5 gives an estimate of the relative amount of material remaining at the end of travel time t and thus an estimate of the fraction of the initial material transported a distance of travel time t. The fraction of pollutant removed by the elimination processes is

$$f_e = 1 - \frac{C}{C_o} = 1 - \exp - \left\{ \frac{\sum_i k_i * t}{1 + K * S} \right\} \quad (11)$$

The fraction of pollutant entering the water that is sorbed to suspended sediment at the end of travel time t is

$$f_s = \frac{K * S * C}{(1 + K * S)} \frac{1}{C_o} = \frac{K * S}{1 + K * S} \exp - \left\{ \frac{\sum_i k_i * t}{1 + K * S} \right\} \quad (12)$$

The fraction of pollutant entering the water that is dissolved at the end of travel time t is

$$f_o = \frac{C}{1 + K * S} \frac{1}{C_o} = \frac{1}{1 + K * S} \exp \left\{ - \frac{\sum_i k_i * t}{1 + K * S} \right\} \quad (13)$$

The fraction of the pollutant eliminated by rate process j is

$$f_{ej} = \frac{\int_o^t k_j * C * dt}{C_o} = \frac{k_j (1 + K * S)}{\left(\sum_i k_i \right)} \left\{ 1 - \exp - \left\{ \frac{\sum_i k_i * t}{1 + K * S} \right\} \right\} \quad (14)$$

For all river calculations, the screening procedure assumes a travel time of 5 days. This travel time was selected because it represents lengths of river reaches between 50 and 250 miles according to the velocities reported by Zison et al. [2]. Contamination of this length of river reach was deemed to be significant.

For pollutant movement and degradation in ponds and lakes, the procedure assumes that a steady state mass balance in a well mixed water body adequately estimates transport and degradation phenomena. This steady state mass balance in equation form is

$$\dot{V} * C_{in}^T = \dot{V} * C^T + V * \left(\sum_i k_i \right) C + C * D \quad (15)$$

where

C_{in}^T = total mass pollutant, dissolved and sorbed per unit volume of influent water
C^T = total mass of pollutant, dissolved and sorbed per unit volume of lake and effluent water
$\dot{V}$ = volume flowrate of water through the lake or pond

V = volume of water in the lake or pond
C = concentration of dissolved pollutant in the lake and lake effluent
D = deposition rate of sorbed pollution per unit volume of water

Solving eqn 10 for the ratio of C^T to C^T_{in} yields

$$\frac{C^T}{C^T_{in}} = \frac{(K \cdot S + 1)(1 - Dt/C^T_{in})}{t \cdot \sum_i k_i + K \cdot S + 1} \quad (16)$$

where

t = average residence time equals $V/\dot{V}$

Furthermore, if we assume that the rate of deposition is proportional to inlet sorbed pollutant concentration,

$$D = N \cdot C^T_{in} \cdot \frac{\dot{V}}{V} \cdot \frac{K \cdot S_{in}}{1 + K \cdot S_{in}} \quad (17)$$

where

N = particulate trap efficiency
S_{in} = sediment concentration in inlet water

If sorbed pollutant and sediment trapping coefficient are identical, the inlake sediment concentration is related to S_{in} as follows:

$$S = (1 - N) \cdot S_{in} \quad (18)$$

Substituting eqns 17 and 18 into equation 16 yields:

$$\frac{C^T}{C^T_{in}} = \frac{(1 + K \cdot S)}{1 + K \cdot S + \left(\sum_i k_i\right) \cdot t} \left\{1 - \frac{K \cdot S \cdot N}{1 - N + K \cdot S}\right\} \quad (19)$$

Simple algebraic operations give expressions for the following ratios:

$$f_e = \frac{\left(\sum_i k_i\right) \cdot t}{1 + K \cdot S + \left(\sum_i k_i\right) \cdot t} \left\{1 - \frac{K \cdot S \cdot N}{1 - N + K \cdot S}\right\} \quad (20)$$

$$f_o = \frac{1}{1 + K \cdot S + \left(\sum_i k_i\right) \cdot t} \left\{1 - \frac{K \cdot S \cdot N}{1 - N + K \cdot S}\right\} \quad (21)$$

$$f_s = \frac{K \cdot S}{1 + K \cdot S + \left(\sum_i k_i\right) \cdot t} \left\{1 - \frac{K \cdot S \cdot N}{1 - N + K \cdot S}\right\} + \frac{K \cdot S \cdot N}{1 - N + K \cdot S} \quad (22)$$

and

$$f_{ri} = \frac{k_i \cdot t}{1 + K \cdot S + \left(\sum_i k_i\right) \cdot t} \left\{1 - \frac{K \cdot S \cdot N}{1 - N + K \cdot S}\right\} \quad (23)$$

where

f_e = fraction of emitted pollutant that is degraded or eliminated
f_o = fraction of emitted pollutant that is dissolved

f_s = fraction of emitted pollutant that is sorbed
f_n = fraction of emitted pollutant that is degraded or eliminated by the ith process

If standing fish crop, $\overline{F}$, and biomass turnover rates are known, then we can use eqn 8 to yield

$$f_f = \frac{k_f \bullet t}{1 + K \bullet S + \left(\sum_i k_i\right) \bullet t} \left\{1 - \frac{K \bullet S \bullet N}{1 - N + K \bullet S}\right\} \quad (24)$$

where

$k_f = k^f \bullet B_f \bullet \overline{F}$
f_f = fraction of emitted pollutant that is taken up by fish

Model parameters estimation procedure

The environmental characteristics of soils, rivers, ponds and reservoirs and compound-specific rate and equilibrium coefficients must be established before the equations presented in the previous section can be used. A summary of soil environmental characteristics that were used in the evaluation of approximately 193 chemicals is shown in Table 1. Literature values, when readily available, were used to describe soil environmental characteristics. When literature values were not available, values were assigned that, according to our technical judgment, would yield a reasonable worst case analysis.

For landfills, the vertical water flux, $\overline{V}$, was set equal to net recharge rate. High and low estimates were based on published data reported by Stewart et al. [3] and represent the expected range of percolation among combinations of soils, rainfall and evapotranspiration rates. The range of velocities of groundwater movement away from landfills was set equal to $\overline{V}$. In actuality these velocities will be larger. As we show in the results section, however, the results of the analysis are relatively insensitive to relatively large errors in groundwater velocities.

A summary of relevent data defining river, pond and reservoir environments is given in Table 2. These values are representative of typical water bodies throughout the country. A range was provided to give reasonable coverage of the possible configurations.

The reaeration rates given in Table 2 were taken directly from Zison et al. [2] or estimated based upon the following relationship.

$$k_{O_2} = \frac{D_{O_2} \bullet 10^5}{(200 \cdot 60 \sqrt{V_w D})} \quad (25)$$

where

Table 1. Environmental characteristics that define groundwater transport

		Reference
Landfill		
Distance to Surface Water	100 m	
Recharge Rate $\overline{V}$-Case 1	0.15 m/yr	Stewart et al. [3]
Recharge Rate $\overline{V}$-Case 2	0.60 m/yr	Stewart et al. [3]
Treatment Lagoon		
Distance to Surface Water	100 m	
H_1	2.4 m	
H_2	1.2 m	
Hydraulic Conductivity $K'h$	96 m/yr	Linsley and Franzinni [16]
Soil porosity, p	0.50	

Table 2. Environmental characteristics of selected water bodies

Water Body	Depth, M	Reaeration Rate Inverse Days	pH	Bulk Sediment Concentration, g/g	Sediment Trap Efficiency	Sediment Organic Matter Con.	Fish Growth Rate, g/g - day
River							
Case 1	5.0[a]	0.22[b]	6.5	50* 10** -6.0[d]	0.00	0.84[e]	1* 10** -8.0[f]
Case 2	1.77[a]	0.93[b]	7.0	1000* 10** -6.0[d]	0.00	0.50[e]	1.69* 10** -7.0[f]
Pond							
Case 1	9.0[a]	0.0593[b]	7.0	50* 10** -6.0[d]	0.89[a]	0.84[e]	1.9* 10** -9.0[f]
Case 2	16.0[a]	0.0334[b]	7.8	1000* 10** -6.0[d]	0.97[a]	0.50[e]	0.06* 10** -6.0[f]
Reservoir							
Case 1	23.0[a]	0.08559[c]	7.0	50* 10** -6.0[d]	0.95[a]	0.84[e]	2.2* 10** -8.0[f]
Case 2	46.0[a]	0.0429[c]	7.8	1000* 10** -6.0[d]	0.99[a]	0.50[e]	1.09* 10** -9.0[f]

References:
[a] Zison et al. [17].
[b] Zison et al. [2].
[c] Perry et al. [18].
[d] Gehm et al. [5].
[e] McElroy et al. [6].
[f] Lagler et al. [8].

D_{O_2} = diffusivity of oxygen, m^2/sec
V_w = wind speed, m/sec
D = depth, m
k_{O_2} = reaeration rate, $days^{-1}$

Reaeration rates were developed for the purpose of estimating pollutant volatilization rates, k_v. Smith et al. [4] have shown that

$$k_v = k_{O_2}(D_m/D_{O_2}) \tag{26}$$

where

D_m = diffusivity of pollutant
D_{O_2} = diffusivity of oxygen

Similarly, Bird et al. [5] have shown that

$$k_v = k_{O_2}(\mathrm{MW}_{O_2}/MW_p) ** 0.5 \tag{27}$$

where

MW_p = molecular weight of pollutant
MW_{O_2} = molecular weight of oxygen

Thus given values for reaeration, k_{O_2}, we can estimate volatilization rate constants for each pollutant. (Note: If the vapor pressure of a compound is less than 0.1 mm Hg, k_v is assumed to be zero. If an estimate of k_v is provided based on data, this value was used with appropriate adjustments for varying depth.)

The bulk sediment concentration and the sediment organic matter content are combined to estimate the effective sediment concentration, S, used in the calculations. The bulk sediment concentrations represent a range of measured values observed in several U.S. rivers as reported by Gehm et al. [5]. Few measurements of the organic matter content of sediments exist, however. Thus a means to estimate the sediment organic matter based upon the more commonly available data for soil organic matter is required. Estimates can be made using the following equation:

$$y = \frac{x}{x + (1 - x)e} \tag{28}$$

where

y = sediment organic matter fraction
x = soil organic matter fraction
e = transport efficiency of soil inorganic matter fraction

This equation was developed assuming that sensibly inorganic matter deposition accounts for all of the difference between sediment release into perennial streams and sediment scoured from the soil surface. By noting that the sediment organic fraction is equal to the amount of organics in sediment divided by the total amount of sediment, the total amount of sediment is equal to the amount of soil organic matter erroded plus the fraction of inorganic matter erroded that is transported to receiving streams, and by dividing each of these amounts by the total amount of sediment erroded, equation 28 directly results.

Based upon observed data within the Yazoo River system, e was calculated to be 0.0101. The equation can be applied to the range of soil organic matter (0 to 5%) reported in McElroy et al. [6] and Buckman and Brady [7]. The sediment-pollutant partition coefficient, K, is scaled to the pollutant-specific octanol/water partition coefficient by the simple relationship

$$K_{om} = 0.25\, K_{ow} \qquad (29)$$

The fish growth rates reported in Table 2 were estimated by multiplying the specific biomass growth rate, 0.01 day ** 0.5, suggested by Zison et al. [2] by typical standing fish crop values reported by Lagler [8] as shown in Table 3. Because the values of Table 3 are given on an areal basis, it is necessary to adjust for the depths chosen for each case.

Table 3. Fish standing crop

Water Body	Range gm** -2.0	Conservative Avg. gm** -2.0
River	5-30	8
Oligotrophic lake	1-5	3
Eutrophic lake	30-280	50

The partition coefficient for the fish, K', is related to properties of the pollutant via the following equation from Neely [9]:

$$K' = 0.59 * K_{ow} ** 0.75 \qquad (30)$$

To use the screening procedure, data on physical and chemical properties must be collected for each compound. This step is the most resource intensive activity required for the conduct of the assessment. The procedure is structured to provide exposure estimates in the face of data gaps. If degradation data are not available, partition calculations can still be made if vapor pressure and solubility or Henry's law coefficients and sediment/water partition coefficients are known. For many organic compounds, sediment/water partition coefficients can be estimated from octanol/water partition coefficients.

In the analysis of 193 compounds, molecular weights, vapor pressures, and solubilities were obtained from standard references, such as the *Handbook of Chemistry and Physics* [10], the *Handbook of Environmental Data on Organic Chemicals* [11], and the *Herbicide Handbook* [12]. If the structural formulas were known, values of octanol/water partition coefficients were estimated using a group contribution method developed by Hansch and Leo [13].

If solubility is not known but octanol/water partition coefficient is known, the correlation developed by Chiou et al. [14]

$$\log S = 7.5 - 1.5 * \log K_{ow} \qquad (31)$$

where

S = solubility (μ mol/L)
K_{ow} = octanol/water partition coefficient

can be used to estimate solubility. Obviously, if the solubility is known and K_{ow} is not known, this same correlation can be used to estimate K_{ow}.

If degradation data are available, a more complete analysis can be done. In the analysis performed on 193 chemicals, only limited data were found. Much of the data was qualitative, and in many cases, professional judgement had to be used to estimate specific degradation rate coefficients. There appeared to be no general pattern that

would provide a basis for concentrating a literature search for degradation data. One simply had to search as much of the environmental literature as possible.

RESULTS

For each compound, a range of loading estimates was made and for each water body a range of estimates of fractions of pollutant which are sorbed, transported, degraded, and volatilized was calculated. If the fraction calculated for a category was less than 10%, a qualitative descriptor of "low" was assigned to that category. If the fraction calculated was between 10% and 80%, a qualitative descriptor of "significant" was assigned. If the fraction calculated was greater than 80%, a qualitative descriptor of "high" was assigned.

The fraction bioaccumulated was also calculated. If the bioaccumulation factor was less than 100 for this parameter, however, a qualitative descriptor of "low" was assigned. If it was between 100 and 1000, a qualitative descriptor of "significant" was defined. If it was above 1000, a qualitative descriptor of "high" was assigned.

A computer program was written to perform all calculations, assign descriptors, and type a text that used the descriptors to qualitatively describe the potential exposure potential of each chemical. A sample of typical output for one of the 193 chemicals analyzed is:

5 ACETOPHENONE

The potential release rates of ACETOPHENONE from storage, treatment, or disposal sites depend upon its chemical properties; the type, location, design and management of the storage, treatment, or disposal systems; and the environmental characteristics of the release site. The estimated potential release rates presented here are based on an evaluation of properties of ACETOPHENONE that determine its movement from unconfined landfills and lagoons and on an estimation of parameters that reflect possible landfill and lagoon configurations. The estimated potential release rates of ACETOPHENONE can be used to assess the magnitude of its potential to contaminate groundwater and as sources for the aquatic exposure assessment included in this report.

ACETOPHENONE was found to be a contaminant in at least one waste stream. The unit release rate to surface waters was estimated to be from *15* mg per square meter of surface area per fraction of the waste stream per year to *62* mg per square meter of surface area per fraction of the waste stream per year for landfills and *230* mg per linear meter adjacent to surface water per fraction of the waste streams per year for lagoons. Approximately *100*% of the material emitted from a landfill is estimated to reach surface waters. Approximately *100*% of the material emitted from a lagoon is estimated to reach surface waters.

Movement of ACETOPHENONE downstream from points of discharge in rivers is projected to be *significant*. Based on the analysis performed, between *62*% and *70*% of the amount emitted into the river will be transported a distance of 5 days travel time (approximately 50 to 250 miles). The potential for degradation or elimination of this compound from a river reach traversed in 5 days is *significant*, ranging from *30*% to *38*% of the total amount emitted. The projected amount of dissolved ACETOPHENONE in a river reach traversed in 5 days is *significant*, ranging from 62% to *70*% of the total amount emitted.

The potential for contamination of bottom sediments deposited in river reaches receiving ACETOPHENONE is *low*. Concentration in the sediment may be *9.7* times as great as ambient water concentration. Based on the analysis performed, approximately *0.28*% of the amount emitted will be sorbed to suspended sediments contained within a river reach traversed in 5 days (50 to 250 miles). The potential for bioaccumulation in river reaches receiving ACETOPHENONE is *low*. Based on the analysis performed, approximately *0.000039*% of the amount emitted will be taken up by fish. Concentrations of ACETOPHENONE in fish may be *9.2* times as great as dissolved concentrations. Estimated potential release to the atmosphere from a river reach traversed in 5 days (50 to 250 miles) is *significant* ranging from *3.1*% to *12*%.

The following table provides examples of actual data, from chemical analysis, listed in EPA's Distribution Register of Organic Pollutants in Water (Water DROP) as described by Garrison et al. [15]. Data are listed for only the categories raw drinking water, finished drinking water, surface water and well water.

Reported Observations of Acetophenone 5 in Major Media Categories

Sample Description	Maximum Concentration Reported (μg/L)	Reference
Surface water	41	1

1. *Journal of the Water Pollution Control Federation*, 35, 777 (1963)

The underlined numbers and words are taken from the computer file for each compound. The output printed here define the behavior of acetophenone in rivers. The complete output, including descriptive behavior of acetophenone in ponds, lakes, and reservoirs, can be obtained from the authors.

In addition to the qualitative evaluations, observations of the occurrence of compound in the environment are strong evidence that the compound is persistant. In conjunction with the use of our evaluation procedure, we screened the Distribution Register of Organic Pollutants in Water (Water DROP) for such data.

Water DROP is an interactive computerized data base of information about organic compounds identified as pollutants in all types of water (e.g., drinking water, surface water, industrial effluents, etc.) as described by Garrison et al. [15]. Information for Water DROP is obtained from published reports, government documents, laboratory reports, and personal communications. For each occurrence, the data base contains a citation that includes compound name, Chemical Abstracts Service Registry Number (CASRN), sample water type, sampling method, sampling site, sampling date, analytical method, concentration detected, analytical laboratory, data quality indicator, and a reference to the data source. Citations can be retrieved on remote terminals by any one of the data elements. Water DROP is a part of the EPA/NIH Chemical Information System (CIS) and is available to CIS subscribers all over the world.

This data base is still being developed and expanded. In January 1980 it contained 10,500 citations containing information about 1700 unique compounds. It must be kept in mind that the number of times that a substance is reported in Water DROP does not necessarily indicate its distribution in the environment; occurrence in Water DROP is influenced by whether or not and how extensively the compound was monitored. Conversely, the absence of a compound from Water DROP does not guarantee its absence from ambient waters; the water may not have been analyzed by a technique that would have detected the chemical. In general, the potential for human exposure can be considered high for any compound reported frequently in Water DROP.

As part of the screening procedure, a sensitivity analysis was done on each of the seven model parameters that potentially affected the transport and persistance of pollutants in surface waters. These parameters are:

1. Octanol/water partition coefficient
2. Hydrolysis rate coefficient
3. Photolysis rate coefficient
4. Bacterial degradation rate coefficient
5. Oxidation rate coefficient
6. Overall degradation rate coefficient
7. Volatilizaton rate

Initially, the model was run with no changes in any of these seven input parameters to establish a base file for comparison purposes. The output contained in this file consisted of a compound name and a set qualitative descriptor for each compound. Table 4 shows the base qualitative descriptor distribution.

Each of the seven parameters were increased and decreased by factors of 10 to 100. Model simulations were run for each

Table 4. Distribution of qualitative descriptors for 193 compounds analyzed

Type of Process	Qualitative Indicator		
	Low	Significant	High
Hydrolysis	306	95	85
Bacterial degradation	790	345	251
Photolysis	60	41	25
Oxidation	54	16	20
Non-process specific degradation	327	169	134
Partitioning without degradation	247	276	197
Total	1784	942	712

Table 5. Results of sensitivity analysis

Multiplication Factor	Results of Sensitivity Analysis Descriptor Changes Expressed as Percent of Total Sample Parameters					
	Partition Coefficient	Hydrolysis Rate Coef.	Bacterial Degradation Rate Coef.	Photolysis Rate Coef.	Overall Rate Coef.	Volatilization Rate Coef.
0.01	8.8	31.3	31.5	29.4	34.9	19.1
0.10	6.5	23.5	22.0	21.4	25.1	14.7
10.00	12.7	14.0	19.1	25.5	22.5	14.9
100.0	24.4	23.3	22.9	30.2	28.9	17.7

parameter value. It should be noted that as the value of one parameter was changed, the other six parameters were held constant at their base values.

Output descriptors for each sensitivity run were compared to the base file key descriptors. Descriptor changes were expressed as a percentage of total base sample for each parameter. For example, if 28 compounds hydrolyzed and there are 18 descriptors per compound, 504 descriptors could change as a result of changing hydrolysis rate coefficients. If 18 of these keywords changed when hydrolysis rate coefficients were increased by a factor of 10, 3.6% of the total sample would change.

Results of the sensitivity analysis are summarized in Table 5. As this table indicates, the most sensitive parameter is the overall degradation rate coefficient. Hydrolysis, bacterial degradation and photolysis rate coefficients are almost as sensitive as the overall degradation rate coefficient.

The volatilization rate coefficient and the partition coefficient are less sensitive parameters. With the exception of the partition coefficient, variation of parameter values translate to roughly symmetric variation in descriptor changes as shown in Figures 2 and 3. Increasing the partition coefficient values, however, causes a greater number of changes than decreasing values. This occurs because initial estimates of partition coefficients were such that most

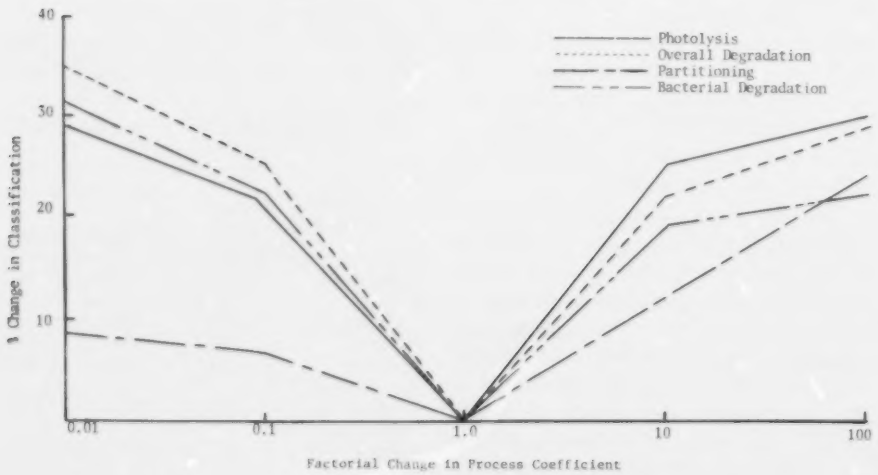

Fig. 2. Change in keywords descriptors versus changes in process coefficient.

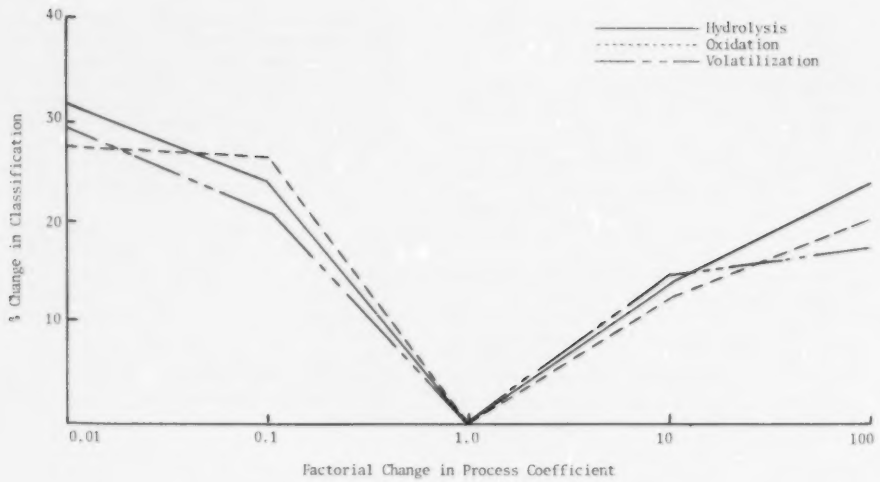

Fig. 3. Change in keyword descriptors versus changes in process coefficient.

chemicals analyzed were largely dissolved rather than sorbed. Thus, decreasing the partition coefficient noticeably increases the dissolved fraction of only a few constituents. On the other hand, increasing the partition coefficient increases the sorbed fraction of many constituents.

The model results are insensitive to variation in groundwater velocity. For any sensible hydrolysis rate, virtually all of the pollutant is degraded before moving 100 meters from the point of discharge for a range of groundwater velocities between 0 and 10 meters per year as illustrated in Figure 1. Given a hydrolysis rate coefficient of 1.9×10^{-3} day^{-1} for velocities below 10 meters per year, more than 97% of the emitted pollutant is degraded before moving 100 meters. A value of 1.9×10^{-3} day^{-1} is the smallest hydrolysis rate coefficient estimated. For higher rate coefficients greater amounts of pollutant would be degraded. Consequently, a pollutant is virtually completely degraded within 100 meters of discharge for any sensible rate coefficient and for any reasonable range of groundwater velocities. Obviously when hydrolysis does not occur, all of the pollutant emitted is eventually transported 100 meters.

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